

CHEMICAL STUDY AND BIOACTIVE POTENTIAL OF THE SPECIES *Vitex orinocensis* Kunth. (Lamiaceae)

Juliene Aljahara Sousa Cardoso^{1*}, Aramys Silva dos Reis², Ivaneide Oliveira Nascimento⁴,
Antônio José Cantanhede Filho¹, Juliana Aljahara Sousa do Nascimento³, Ana Karlla dos
Santos Sousa², Maria de Fátima das Graças Fernandes da Silva⁵, Alan Bezerra Ribeiro²

jullienecardoso@gmail.com

1-Departamento de Química, Instituto Federal de Educação, Ciência e Tecnologia, Av. Getúlio Vargas, Campus Monte Castelo, São Luís, Maranhão, 65030-005, Brazil. 2-Centro de Ciência de Imperatriz, Universidade Federal do Maranhão, Campus Imperatriz, Imperatriz, Maranhão, 65900-410, Brazil. 3-Centro de Biociências, Universidade Federal de Pernambuco, Av. Professor Moraes, Recife, Pernambuco, 50670-420, Brazil. 4-Centro de Ciências Exatas, Naturais e Tecnológicas, Universidade Estadual da Região Tocantina do Maranhão, Brazil. 5-Universidade Federal de São Carlos, Rodovia Washington Luís, km 235, São Carlos, São Paulo, 13565-905

Vitex orinocensis Kunth is a native tree species from South America traditionally used in Brazilian folk medicine, especially in Maranhão state. Despite its ethnobotanical relevance, no phytochemical or biological data had been available in the scientific literature prior to this work. This study aimed to perform a comprehensive phytochemical investigation of the bark of *V. orinocensis* and to evaluate its potential against *Leishmania amazonensis*, the etiological agent of cutaneous leishmaniasis. Crude extracts were obtained by sequential solvent extraction (hexane, ethyl acetate, and methanol). The ethyl acetate was selected chromatographic fractionation using silica gel column chromatography. The isolation of secondary metabolites were performed by preparative high-performance liquid chromatography (HPLC), and compound structures were elucidated based on 1D and 2D Nuclear Magnetic Resonance (¹H and ¹³C NMR), supported by literature data. This approach allowed the isolation of four pentacyclic triterpenes, namely (3 β)-Olean-12-en-3-ol, (3 β)-3-Hydroxyurs-12-en-28-oic acid, (3 β)-3-Hydroxyolean-12-en-28-oic acid, and (3 β ,11 β)-dihydroxyurs-12-ene. The crude extracts were then tested against promastigote forms of *L. amazonensis*. The hexane and ethyl acetate extracts showed significant antiparasitic activity, with IC₅₀ values of 46.17 μ g/mL and 47.48 μ g/mL, respectively. In addition, cytotoxicity assays using RAW 264.7 macrophage cells revealed CC₅₀ values >240 μ g/mL for both extracts. Selectivity Index (SI) values of 5.23 (hexane) and 4.43 (ethyl acetate) suggest selective action against the parasite with low toxicity to host cells. Conversely, the methanolic extract exhibited low activity (IC₅₀ > 400 μ g/mL) but was non-toxic to mammalian cells (CC₅₀ > 400 μ g/mL), indicating potential utility in combination therapies. This is the first report on the chemical profile and antileishmanial effects of *V. orinocensis*, supporting its traditional use and highlighting its potential for phytopharmaceutical development.

Keywords: *Vitex orinocensis*, triterpenes, bioactivity, *L. amazonensis*

